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Influence of molecular-scale roughness on the surface spreading of an aqueous nanodrop[1] ALENKA LUZAR, Department of Chemistry, Virginia Commonwealth University, C.D. DAUB, J. WANG, S. KUDESIA, D. BRATKO —
We study the spreading of an aqueous nanodrop on a smooth surface decorated by sub-nanoscale asperities at varied surface coverage and with different distribution patterns. Using molecular dynamics simulations, we consider two substrate materials, a hydrophilic and a hydrophobic one. Interestingly, the introduction of surface asperities gives rise to a sharp increase in the apparent contact angle on *both* types of surfaces. The superhydrophobic state with the maximal contact angle of 180 degrees is reached when the asperity coverage on a hydrophobic substrate is below 25%, suggesting that superhydrophobicity can also be achieved by nanoscale roughness of a macroscopically smooth material. We further examine the effect of surface roughness on droplet mobility on the substrate. The apparent diffusion constant shows a dramatic slowdown of the nanodroplet translation even for asperity coverage in the range of 1% for hydrophilic surface, while droplets on corrugated hydrophobic surfaces retain the ability to flow around the asperities. In contrast, for smooth surfaces we find that the drop mobility on the hydrophilic surface exceeds that on the hydrophobic one.

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Alenka Luzar
Department of Chemistry, Virginia Commonwealth University

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